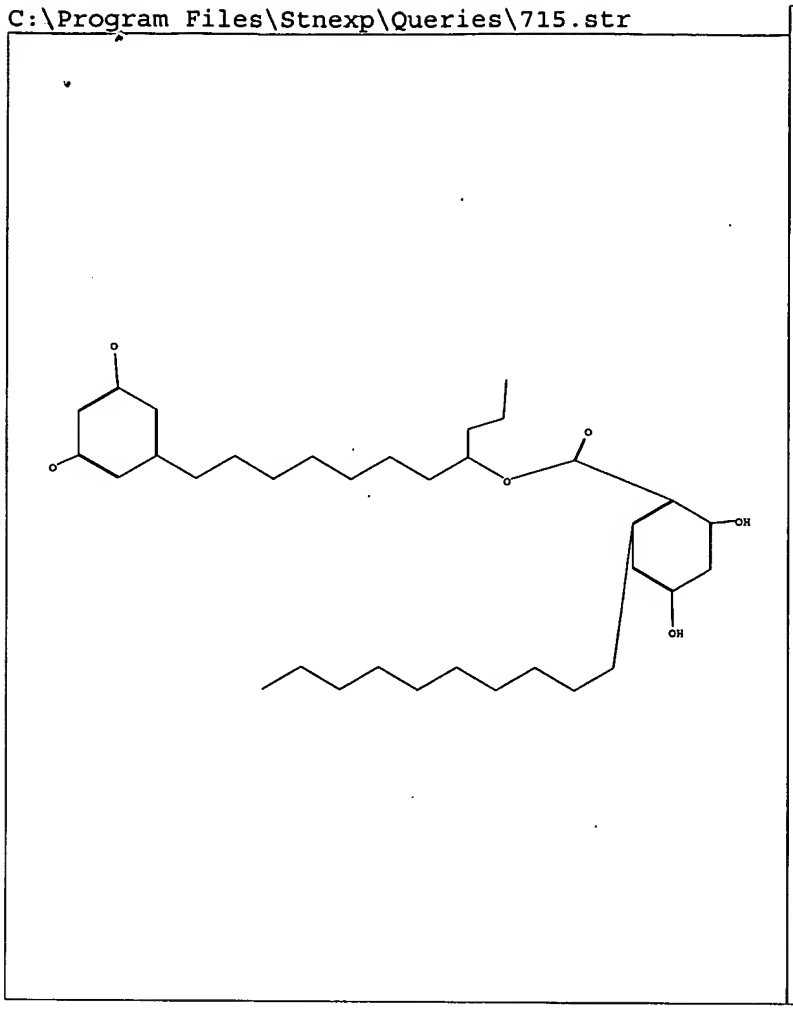
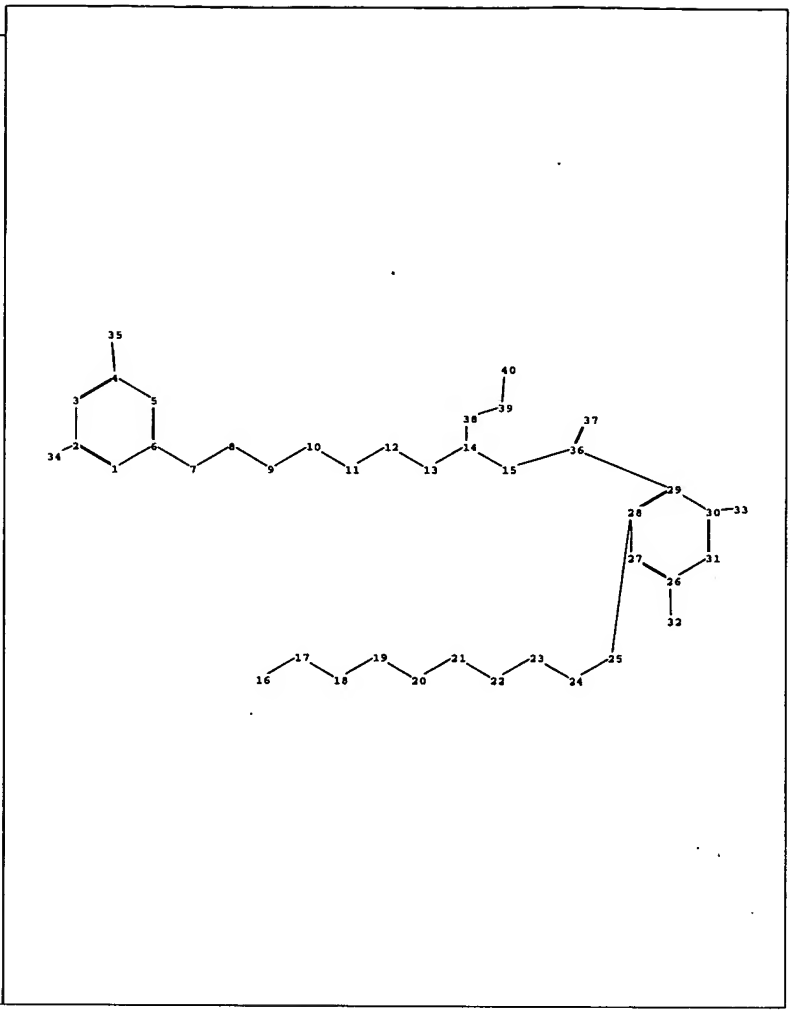
C:\Program Files\Stnexp\Queries\715.str





chain nodes :
7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 32 33 34 35 36 37 38 39 40
ring nodes :
1 2 3 4 5 6 26 27 28 29 30 31
chain bonds :
2-34 4-35 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15 14-38 15-36 16-17 17-18 18-19 19-20 20-21 21-22 22-23 23-24 24-25 25-28 26-32 29-36 30-33 36-37 38-39 39-40
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 26-27 26-31 27-28 28-29 29-30 30-31
exact/norm bonds :
2-34 4-35 14-15 15-36 26-32 30-33 36-37
exact bonds :
6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-38 16-17 17-18 18-19 19-20 20-21 21-22 22-23 23-24 24-25 25-28 29-36 38-39 39-40
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 26-27 26-31 27-28 28-29 29-30 30-31

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS

```
Uploading C:\Program Files\Stnexp\Queries\715.str

L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 full
   REGIstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.




FULL SEARCH INITIATED 16:40:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      788 TO ITERATE

100.0% PROCESSED      788 ITERATIONS                                5 ANSWERS
SEARCH TIME: 00.00.01

L2             5 SEA SSS FUL L1



L3           5 L2

=> s l3 and py<2003
      22789434 PY<2003
L4           2 L3 AND PY<2003

=> d 1-2 ibib abs hitstr

L4   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2002:136800  CAPLUS
DOCUMENT NUMBER:          137:2812
TITLE:                    Discovery, structure and HIV-1 integrase inhibitory
                          activities of integracins, novel dimeric alkyl
                          aromatics from Cytonaema sp.
AUTHOR(S):                Singh, Sheo B.; Zink, Deborah L.; Bills, Gerald F.;
                          Pelaez, Fernando; Teran, Ana; Collado, Javier;
                          Silverman, Keith C.; Lingham, Russell B.; Felock,
                          Peter; Hazuda, Daria J.
CORPORATE SOURCE:         Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE:                   Tetrahedron Letters (2002), 43(9), 1617-1620
                          CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER:                Elsevier Science Ltd.
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
GI
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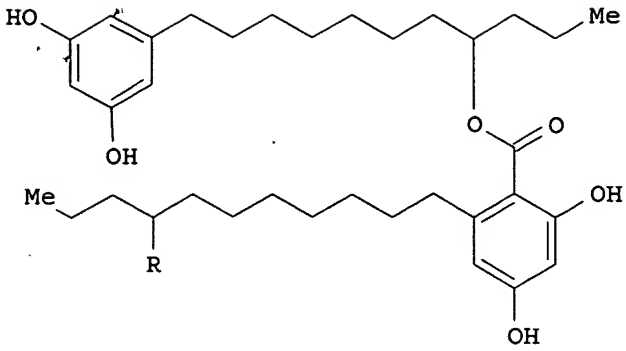
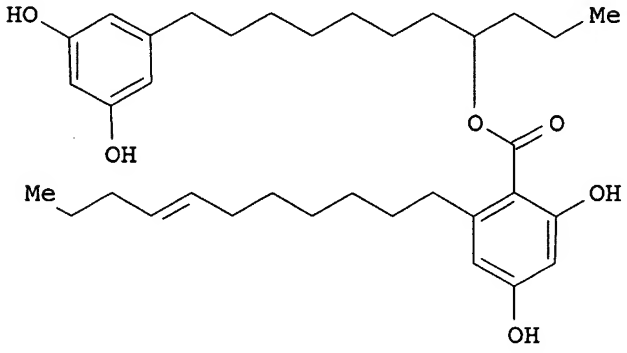


I R=OAc
II R=OH



III

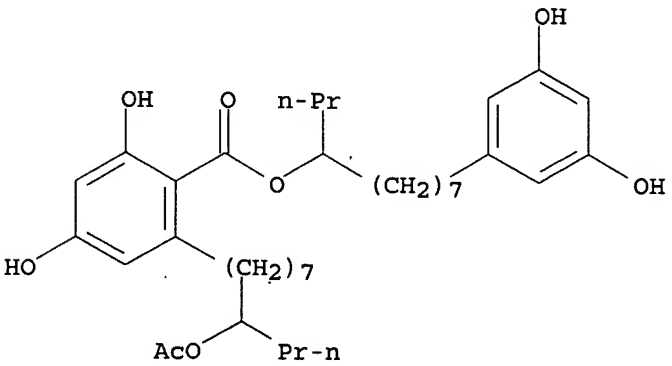
AB Integrase is a critical viral enzyme for HIV-1 replication and is a novel target for therapeutic intervention against HIV infections. Integracins A, B, and C (I, II, and III, resp.) are three novel dimeric alkyl aromatic inhibitors of HIV-1 integrase discovered from the screening of fungal exts. using an in vitro assay. These compds. inhibit both coupled and strand transfer activity of HIV-1 integrase with IC50 values of 3.2-6.1 and 17-88 μM, resp. The discovery, structure and activity of these compds. are described.

IT **224186-03-2P**, Integracin A **224186-05-4P**, Integracin B
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)
(discovery, structure, and HIV-1 integrase inhibitory activities of integracins from Cytonaema)

RN 224186-03-2 CAPLUS

CN Benzoic acid, 2-[8-(acetyloxy)undecyl]-4,6-dihydroxy-, 8-(3,5-dihydroxyphenyl)-1-propyloctyl ester (9CI) (CA INDEX NAME)

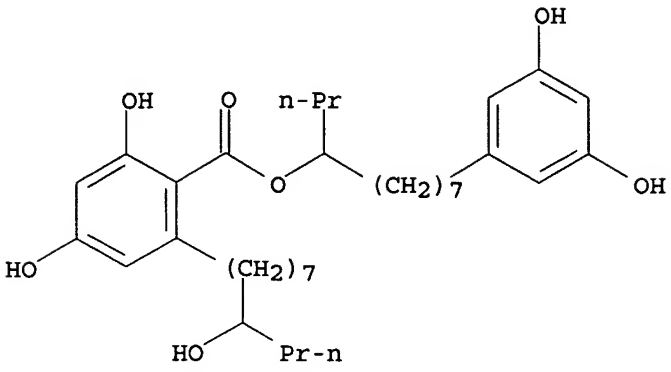
Rotation (-).
Currently available stereo shown.



RN 224186-05-4 CAPLUS

CN Benzoic acid, 2,4-dihydroxy-6-(8-hydroxyundecyl)-, 8-(3,5-dihydroxyphenyl)-1-propyloctyl ester (9CI) (CA INDEX NAME)

Rotation (-).
Currently available stereo shown.

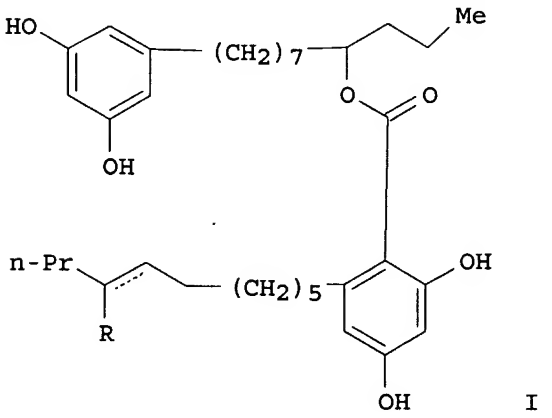


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:341193 CAPLUS
DOCUMENT NUMBER: 130:357144
TITLE: Hydroxyphenylundecanes as HIV integrase inhibitors
INVENTOR(S): Bills, Gerald F.; Lingham, Russell B.; Silverman, Keith C.; Singh, Sheo B.; Teran, Ana; Zink, Deborah L.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Brit. UK Pat. Appl., 40 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
GB 2327674	A1	19990203	GB 1998-15925		19980722	<--
US 6124327	A	20000926	US 1998-123180		19980727	<--
PRIORITY APPLN. INFO.:			US 1997-54074P	P	19970729	
			GB 1998-226	A	19980106	

GI



I

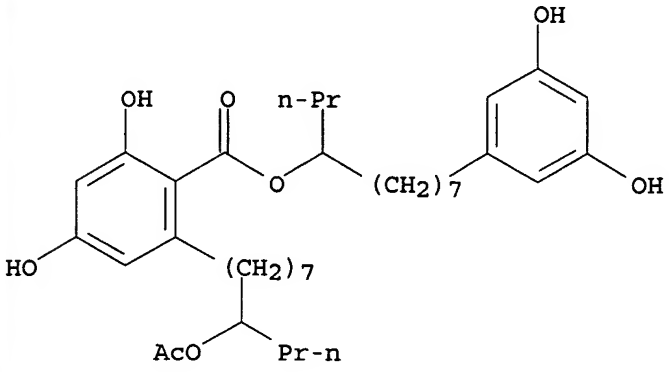
AB A pharmaceutical composition, useful for inhibiting HIV integrase and prevention or treatment of HIV infections, i.e. AIDS and ARC, comprises a dimerized hydroxyphenylundecane (I; R = OH, OC(O)Me) isolated from Cytonaema culture MF6253 (ATCC 74413) in combination with antiviral, anti-infective, and/or immunomodulating agents. Biosynthetic preparation by fermentation of MF6253, isolation, and phys. and spectral properties of three dimerized hydroxyphenylundecanes, as well as an assay of HIV integrase

inhibition by these compds. are presented.

IT **224186-03-2P 224186-05-4P**
RL: BAC (Biological activity or effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(compns. containing hydroxyphenylundecanes as HIV integrase inhibitors for treatment of HIV infections)

RN 224186-03-2 CAPLUS
CN Benzoic acid, 2-[8-(acetyloxy)undecyl]-4,6-dihydroxy-, 8-(3,5-dihydroxyphenyl)-1-propyloctyl ester (9CI) (CA INDEX NAME)

Rotation (-).
Currently available stereo shown.



RN 224186-05-4 CAPLUS
CN Benzoic acid, 2,4-dihydroxy-6-(8-hydroxyundecyl)-, 8-(3,5-dihydroxyphenyl)-1-propyloctyl ester (9CI) (CA INDEX NAME)

Rotation (-).
Currently available stereo shown.